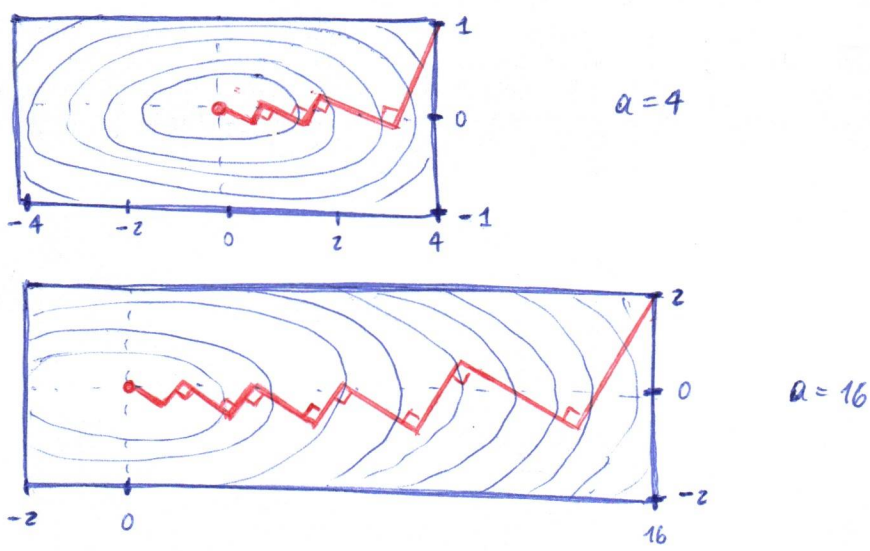
Gradient Method

Unconstrained Nonlinear Optimization

- The gradient method is a method for unconstrained optimization problems ($\min\{f(\underline{x}) : \underline{x} \in \mathbb{R}^n\}$) based on the search directions defined by the gradient of the function at the current point.
- Given a $\mathcal{C}^1$ function $f : \mathbb{R}^n \to \mathbb{R}$, we look for a stationary point. We start from a $\underline{x}_0$ and we set $k = 0$. At the k-th iteration we set $\underline{d}_k = -\nabla f(\underline{x}_k)$ and we determine $\alpha_k > 0$ by solving (exactly) the 1-D problem $\min_\alpha \phi(\alpha) = f(\underline{x}_k + \alpha \underline{d}_k)$ (we choose a directoin and we minimize along it). Then we move at $\underline{x}_{k+1} = \underline{x}_k + \alpha_k \underline{d}_k$ and we repeat. We go on untill we match one termination criteria: $||\nabla f(\underline{x}_k)|| < \epsilon$, $|f(\underline{x}_{k+1}) - f(\underline{x}_k)| < \epsilon$, $||\underline{x}_{k+1} - \underline{x}_k|| < \epsilon$.

  Notice: if the 1-D is exact, the successive directions are orthogonal. This may not be good for the convergence speed: zig-zag trajectories have a slow convergence.
- For quadratic strictly convex function $f(\underline{x}) = \frac{1}{2}\underline{x}^T Q \underline{x} - \underline{b}^T \underline{x}$, with Q symmetric and positive definite, the global minimum is the unique solution of $\nabla f(\underline{x}) = Q\underline{x} - \underline{b} = \underline{0}$, and so α_k can be determined explicitly as: $\alpha_k = \frac{\underline{d}_k^T \underline{d}_k}{\underline{d}_k^T Q \underline{d}_k}$ (with $\underline{d}_k = \nabla f(\underline{x}_k)$).
- **Convergence.** For quadratic strictly convex functions $f \in \mathcal{C}^2$ we have that the method is globally convergent (for all $\underline{x}_0$ the $\lim_{k\to\infty} \underline{x}_k = \underline{x}^*$) and $||\underline{x}_{k+1} - \underline{x}^*||_Q^2 \leq (\frac{\lambda_n - \lambda_1}{\lambda_n + \lambda_1})^2 ||\underline{x}_k - \underline{x}^*||_Q^2$, where $0 < \lambda_1 \leq \lambda_2 \leq .. \leq \lambda_n$ are the eigenvalues of Q. If the spectrum of Q is small (λ_1 close to λ_n) then the rate will be small. Smaller the spectrum, faster the convergence. If $\lambda_1 = \lambda_n$ the method converges in one iteration.
- The method can be extended to arbitrary non linear functions.
  If $f \in \mathcal{C}^2$ and the gradient method with exact 1-D converges to $\underline{x}^*$ with $\nabla^2 f(\underline{x}^*)$ positive definite then $f(\underline{x}_{k+1}) - f(\underline{x}^*) \leq (\frac{\lambda_n - \lambda_1}{\lambda_n + \lambda_1})^2 (f(\underline{x}_k) - f(\underline{x}^*))$, where $0 < \lambda_1 \leq \lambda_2 \leq .. \leq \lambda_n$ are the eigenvalues of $\nabla^2 f(\underline{x}^*)$. Here the convergence is in terms of $f(\underline{x}_k)$ but, since $\nabla^2 f(\underline{x}^*)$ is positive definite, looking at the speed of convergence of $|f(\underline{x}_k) - f(\underline{x}^*)| \to 0$ or $||\underline{x}_k - \underline{x}^*|| \to 0$ is the same.
- **Advantages and disadvantages.** This method has many advantages: is very simple, very light computationally and globally convergent. However, a disadvantage is that the convergence might be very slow (also due to the orthogonality between directions). Moreover, we can see how this method is strongly affected by the structure of the Hessian matrix in $\underline{x}^*$.
- **Deal with disdvantages.** A way to circumvent these disadvantages is to applay the conjugate direction method. This method is based on the search directions $\{\underline{d}_i\}_i$ mutually Q-conjugate ($\underline{d}_i^T Q \underline{d}_j = 0$) with Q $n \times n$ matrix. In this method the search for the optimum procedes one conjugate direction at the time: at the k-th iteration we find the optimal solution in the space spanned by the first k directions. This method guarantees a convergence in at most n step.
- **Example.** $\min f(\underline{x}) = f(x_1, x_2) = \frac{1}{2}x_1^2 + \frac{a}{2}x_2^2$ with $a \geq 1$ and hence eigenvalues $\frac{1}{2}$ and $\frac{a}{2}$.



Newton Method (& Quasi-Newton Methods)

Unconstrained Nonlinear Optimization

- The Newton method is a method for unconstrained optimization problems ($\min\{f(\underline{x}) : \underline{x} \in \mathbb{R}^n\}$). The idea is to extract more information from the objective function than just the linear approximation (gradient method): we approximate f at $\underline{x}_k$ with a quadratic function.
- Given a $\mathcal{C}^2$ function $f : \mathbb{R}^n \to \mathbb{R}$ and its Hessian matrix $H(\underline{x}) = \nabla^2 f(\underline{x})$, we consider the quadratic approximation of $f(\underline{x})$ at $\underline{x}_k$: $q_k(\underline{x}) = f(\underline{x}_k) + \nabla^T f(\underline{x}_k)(\underline{x} - \underline{x}_k) + \frac{1}{2}(\underline{x} - \underline{x}_k)^T H(\underline{x}_k)(\underline{x} - \underline{x}_k)$ and we choose $\underline{x}_{k+1}$ as a stationary point, namely $\nabla q_k(\underline{x}) \Rightarrow \nabla f(\underline{x}_k) + H(\underline{x}_k)(\underline{x}_{k+1} - \underline{x}_k) = \underline{0}$.
  If $H(\underline{x}_k)$ is not singular, then $H^{-1}(\underline{x}_k)$ exists and $\underline{x}_{k+1} = \underline{x}_k - H^{-1}(\underline{x}_k)\nabla f(\underline{x}_k)$.
  From the informations obtained by the quadratic approximation, starting from $\underline{x}_k$ we follow the Newton direction ($\underline{d}_k = -H^{-1}(\underline{x}_k)\nabla f(\underline{x}_k)$) to reach $\underline{x}_{k+1}$, then we repeat and we go on until convergence.

  If $H(\underline{x}_k)$ is positive definite and $\nabla f(\underline{x}_k) \neq \underline{0}$, then the Newton direction $\underline{d}_k$ is a descent direction.
- **Convergence.** If f is quadratic and strictly convex the global minimum is reached in a single iteration. Generally the method is not globally convergent, but has a very fast local convergence if $\underline{x}_0$ is sufficiently close to the desired solution. More precisely, if (1) $f \in \mathcal{C}^2$, (2) $\underline{x}^*$ is such that $\nabla f(\underline{x}^*) = \underline{0}$ and $H(\underline{x}^*)$ is positive definite, (3) $\exists L > 0$ such that $||H(\underline{x}) - H(\underline{y})|| \leq L||\underline{x} - \underline{y}||$, $\forall \underline{x}, \underline{y} \in N(\underline{x}^*)$, then for $\underline{x}_0$ sufficiently close to the local minimum we have the local quadratic convergence.
- **Advantages and disadvantages.** An advantage of the method is the speed of the convergence. Moreover the method is invariant w.r.t. affine coordinate changes. A disadvantage is that, if $H(\underline{x}_k)$ is not positive definite, $\underline{d}_k$ may not be defined or may be an ascent direction. Moreover, even if the direction is a discent direction, it may increase the value of f if not moderated with a multiplier. For the fact that we have to invert a matrix at every iteration, another disadvantage is the heavy computation.
- **Quasi-Newton methods.** The Quasi-Newton methods are variants of the Newton method where 2nd order derivative informations are extracted from variations in $\nabla f(\underline{x})$ instead of using/inverting $\nabla^2 f(\underline{x})$.
  - **DFP.** We generate a sequence $\{H_k\}_k$ of symmetric positive definite approximations of $[\nabla^2 f(\underline{x}_k)]^{-1}$.
    We approximate f around $\underline{x}_k$: $f(\underline{x}_k + \underline{\delta}) \approx f(\underline{x}_k) + \underline{\delta}^T \nabla f(\underline{x}_k) + \frac{1}{2}\underline{\delta}^T \nabla^2 f(\underline{x}_k)\underline{\delta}$.
    Differentiating (w.r.t. $\underline{\delta}$) we obtain: $\nabla f(\underline{x}_k + \underline{\delta}) \approx \nabla f(\underline{x}_k) + \nabla^2 f(\underline{x}_k)\underline{\delta}$.
    Substituting $\underline{\delta}$ with $\underline{\delta}_k := \underline{x}_{k+1} - \underline{x}_k$ and $\underline{\gamma}_k = \nabla f(\underline{x}_{k+1}) - \nabla f(\underline{x}_k)$ we obtain: $\underline{\gamma}_k \approx \nabla^2 f(\underline{x}_{k+1})\underline{\delta}_k$ and so we determine the secant condition: $H_{k+1}\underline{\gamma}_k = \underline{\delta}_k$.
    Since we want a method which is lighter computationally, we procede by successive updates of H_k. The best way is to add two symmetric matrix of rank 1 each, multiplied by a proportionality coefficient. In this way we obtain the rank two updated formula, the DFP formula.

    The advantage is that, since H_k's are symmetric and positive definite (DFP method preserves the positive definitness if H_0 is positive definite and the curvature condition ($\underline{\delta}_k^T \underline{\gamma}_k > 0 \; \forall k$) is satisfied), we can always well define a direction $\underline{d}_k$, which will be a descent direction. Moreover we have superlinear convergence rate (even if, in general, just locally).
  - **BFGS.** Another way to procede is to generate a sequence $\{B_k\}_k$ of approximations of $\nabla^2 f(\underline{x}_k)$. Following the previous method, we have an adapted secant condition to: $B_{k+1}\underline{\delta}_k = \underline{\gamma}_k$. Using again a the rank two updated formula we obtain B_{k+1}, which is structured in such a way that we can invert it analitically, and so obtaining a sequence of $\{H_k\}_k$ trough the BFGS updated formula.

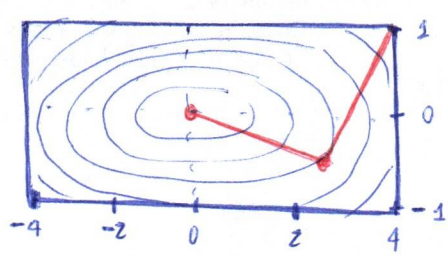
Conjugate Direction Method

Unconstrained Nonlinear Optimization

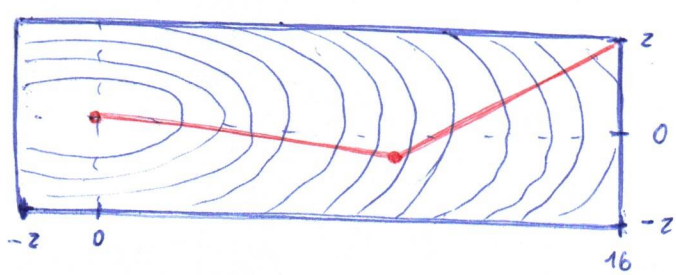
- The conjugate direction method is a method based on the search directions $\{\underline{d}_i\}_i$ mutually Q-conjugate, i.e. $\underline{d}_i^T\, Q\, \underline{d}_j = 0$, with Q $n \times n$ matrix.
- We consider a **quadratic strictly convex function**: $q(\underline{x}) = \frac{1}{2}\underline{x}^T Q \underline{x} - \underline{b}^T \underline{x}$, with $Q \in \mathbb{R}^{n\times n}$ symmetric and positive definite. Since Q is positive definite, the Q-conjugate directions $\{\underline{d}_i\}_i$ are linearly independent. This implies that, if we fix n Q-conjugate directions $\{\underline{d}_i\}_{i=1,..,n}$, the problem of minimize $q(\underline{x})$ is reduced to n 1-D minimization problems.
- For any initial point $\underline{x}_0$, at the k-th iteration we have to minimize the problem $q(\underline{x}_k + \alpha \underline{d}_k)$ along $\underline{d}_k$. Choosing $\alpha_k = -\frac{\underline{g}_k^T \underline{d}_k}{\underline{d}_k Q \underline{d}_k}$, with $\underline{g}_k = \nabla q(\underline{x}_k) = Q\underline{x}_k - \underline{b}$, the sequence $\{\underline{x}_k\}_k$, generated as $\underline{x}_{k+1} = \underline{x}_k + \alpha_k \underline{d}_k$, converges to the unique global optimal solution $\underline{x}^*$ of $q(\underline{x})$ in at most n iterations.
  At every iteration, $\underline{x}_k$ minimizes $q(\underline{x})$ not only on the line $\{\underline{x} \in \mathbb{R}^n : \underline{x} = \underline{x}_{k-1} + \alpha \underline{d}_{k-1},\ \alpha \in \mathbb{R}\}$, but also on the affine subspace $V_k = \{\underline{x} \in \mathbb{R}^n : \underline{x} = \underline{x}_0 + span(\underline{d}_0, .., \underline{d}_{k-1})\}$.
- If the directions $\{\underline{d}_i\}_i$ are not known, at the k-th iteration: $\underline{d}_{k+1} = -\underline{g}_{k+1} + \beta_k \underline{d}_k$, with $\beta_k = \frac{\underline{g}_{k+1}^T \underline{g}_{k+1}}{\underline{g}_k^T \underline{g}_k}$.
- The method can be extended to **arbitrary functions**: we choose α_k with an inexact method, bisection for instance, and we evaluate β_k using famous formulae, for instance Fletcher-Reeves or Polak Ribière:

$$\beta_k^{FR} = \frac{||\nabla f(\underline{x}_{k+1})||^2}{||\nabla f(\underline{x}_k)||^2} \qquad \beta_k^{PB} = \frac{\nabla^T f(\underline{x}_{k+1})(\nabla f(\underline{x}_{k+1}) - \nabla f(\underline{x}_k))}{||\nabla f(\underline{x}_k)||^2}.$$

  We obtain $\underline{d}_{k+1} = -\nabla f(\underline{x}_{k+1}) + \beta_k \underline{d}_k$ and a sequence $\{\underline{x}_k\}_k$: $\underline{x}_{k+1} = \underline{x}_k + \alpha_k \underline{d}_k$.
- **Convergence.** For quadratic strictly convex function we have: $||\underline{x}_{k+1} - \underline{x}^*||_Q^2 \leq (\frac{\lambda_{n-k} - \lambda_1}{\lambda_{n-k} - \lambda_1})^2 ||\underline{x}_0 - \underline{x}^*||_Q^2$, where $0 < \lambda_1 \leq \lambda_2 \leq .. \leq \lambda_n$ are the eigenvalues of Q. If there are m large eigenvalues and $n - m$ concentrated eigenvalues, after $m + 1$ iterations we obtain an accurate estimate of the solution. The method converges in at most n iterations. In the case of arbitrary functions, if we generates β with the FR method we have the global convergence. Moreover, if: $f \in \mathcal{C}^2$, $\{\underline{x}_k\}_k$ generated by FR converges to $\underline{x}^*$ and $\nabla^2 f(\underline{x}^*)$ is positive definite then we have the superlinear convergence in n iterations.
- **Advantages.** This method is better than the Gradient method because it's faster in the convergence. Moreover, this method is better then the Newton method because of the lower computational load: at every iteration we only need to memorize 4 vectors $(\underline{x}_k, \underline{d}_k, \nabla f(\underline{x}_k), \nabla f(\underline{x}_{k+1}))$. Another advantage is the guarancee of the global convergence (for arbitrary functions) through the restart method.
  Disadvantages. This method needs an exact or at least accurate 1-D search, otherwise the directions may loose the Q-conjugacy. Moreover, the method is not invariant with respect to transformations of the coordinates, and so it's not so easy to perform the preconditionament.
- **Example.** min $f(\underline{x}) = f(x_1, x_2) = \frac{1}{2}x_1^2 + \frac{a}{2}x_2^2$ with $a \geq 1$ and hence eigenvalues $\frac{1}{2}$ and $\frac{a}{2}$.



$a = 4$



$a = 16$

Since we are in a 2 dimensional space, we have the optimal solution in at most 2 iterations (↓ how large the spectrum of Q is, so ↓ of how far are $\frac{1}{2}$ and $\frac{a}{2}$ (eigenvalues of Q))

Quadratic Programming

Constrained Nonlinear Optimization

- The quadratic programming method is used to minimize quadratic functions subject to linear constraints: (P) $= \min \{q(\underline{x}) = \frac{1}{2}\underline{x}^T Q\underline{x} + \underline{c}^T\underline{x} : \ \underline{a}_i^T\underline{x} \leq b_i \ i \in I, \ \underline{a}_i^T\underline{x} = b_i \ i \in E, \ \underline{x} \in \mathbb{R}^n\}$ with Q symmetric.
- **Only equalities.** We consider (P^1), only equality constraints: $\min \{q(\underline{x}) = \frac{1}{2}\underline{x}^T Q\underline{x} + \underline{c}^T\underline{x} : \ A\underline{x} = \underline{b}\}$, with $A \in \mathbb{R}^{m\times n}$. We use the null-space method. We determine $Z \in \mathbb{R}^{n\times(n-m)}$ whose columns span the null space of A. Given a feasible direction $\underline{x}_0$, any other feasible solution can be written as $\underline{x} = \underline{x}_0 + Z\underline{w}$, with an appropriate $\underline{w} \in \mathbb{R}^{n-m}$. In this way we can rewrite (P^1) as an unconstrained QP:

$$\min\{\frac{1}{2}\underline{w}^T(Z^TQZ)\underline{w} + (Q\underline{x}_0 + \underline{c}^T)Z\underline{w} : \ \underline{w} \in \mathbb{R}^{n-m}\}.$$

  If Z^TQZ is positive definite $\exists!$ optimal solution $\underline{w}^*$, obtained by solving: $(Z^TQZ)\underline{w} = -Z^T(Q\underline{x}_0 + \underline{c})$.
- **Equalities and inequalities.** We consider now the problem (P) with both equality and inequality constraints. We use the active-set method. The idea behind is that QP with only equality constraints is easier to solve, so we try to transform (P) in a sequence of QP subject to only equality constraints.

  0. We define the working set $W_k \subseteq \{i \in I : \underline{a}_i^T\underline{x}_k = b_i\} \cup E$.
  We start with a feasible solution $\underline{x}_0$ of (P) and we set $k = 0$.

  1. Given the feasible solution $\underline{x}_k$ we look for the direction $\underline{d}_k$ that optimizes the subproblem:
  $\min \{q(\underline{x}_k + \underline{d}) : \ \underline{a}_i^T(\underline{x}_k + \underline{d}) = b_i \ i \in W_k\}$ (equivalent to $\min \{q(\underline{x}_k + \underline{d}) : \ \underline{a}_i^T\underline{d} = 0 \ i \in W_k\}$), where W_k is the current working set.

  2.a If $\underline{d}_k \neq \underline{0}$ we determine the longest step length satisfying all constraints not in W_k:

$$\alpha_k = \min\{1, \min_{i\notin W_k, \ \underline{a}_i^T\underline{d}_k > 0} \frac{b_i - \underline{a}_i^T\underline{x}_k}{\underline{a}_i^T\underline{d}_k}\}$$

  We set $\underline{x}_{k+1} = \underline{x}_k + \alpha_k\underline{d}_k$ and we update $W_{k+1} = W_k \cup \{i'\}$, where i' is the index of the constraint becoming active in $\underline{x}_{k+1}$. Then we go back at **1.**

  2.b If $\underline{d}_k = \underline{0}$, $\underline{x}_k$ not necessarily is the ultimate optimal solution, we only know that it's otpimal in W_k. We set $\underline{x}_{k+1} = \underline{x}_k$ and we determine the multipliers u_i^k from the KKT conditions on W_k:

$$\nabla q(\underline{x}_k) + \textstyle\sum_{i\in W_k} u_i^k\underline{a}_i = \underline{0}$$

  If $u_i^k \geq 0 \ \forall i$ then $\underline{x}_k$ is the local optimum of (P), and we're done. Otherwise, if $\exists\, u_i^k < 0$ then we update $W_{k+1} = W_k \setminus \{i'\}$, where i' is the index of the most negative u_i^k, and we go back to **1.**

  Notice that if $W_k = \emptyset$ then the optimal direction is the steepest descent direction $\underline{d}_k = -\nabla q(\underline{x}_k)$.
- If Q is positive definite ($q(\underline{x})$ is strictly convex) the method finds and optimal solution within a finite number of iterations.
- **Advantages.** As an advantage we have that if the global minimum of the function is strictly inside of X then we reach it in few iterations. Otherwise, if $\underline{x}^* \notin X$ we have to find the best $\underline{x}_k \in X$ that approximate it. Another advantage is that QPs are the simplest NLP problems besides Linear Programs. A direct application is the portfolio optimization.

Penalty Methods

Constrained Nonlinear Optimization

- We consider a generic NLP problem (P): $\min \{f(\underline{x}) : \ c_i(\underline{x}) \geq 0 \ i \in I, \ \ c_i(\underline{x}) = 0 \ i \in E, \ \ \underline{x} \in \mathbb{R}^n\}$, where f and c_i's are $\mathcal{C}^1$ or $\mathcal{C}^2$. The idea behind the quadratic penalty method is to delete constraints and add terms to the objective function which penalize the violation of the constraints. In this way the original optimization problem becomes a sequence of unconstrained optimization problems.
- **Only equalities.** We consider the problem (P^1) with only equality constraints and we define the quadratic penalty function problem associated to (P^1) as: $\min Q(\underline{x}, \mu) = f(\underline{x}) + \frac{1}{2\mu} \sum_{i \in E} c_i^2(\underline{x})$, with the penalty parameter $\mu > 0$. If we want that eventually the equality constraints are really satisfied we need to increase the weight that we assign to the penality, and so we need $\mu_k \to 0$.

0. We select an accuracy parameter $\epsilon > 0$, a starting penalty parameter $\mu_0 > 0$ and a sequence of tolerances $\{\tau_k\}_{\tau \geq 0}$ with $\tau_k \geq 0$ and $\tau_k \to 0$. We choose an initial $\underline{x}_0^{start}$ and we set $k = 0$.

1. Starting from $\underline{x}_k^{start}$ we determine an approximate minimizer $\underline{x}_k$ of $Q(\underline{x}_k, \mu_k)$ with the stopping criterium: $||\nabla Q(\underline{x}, \mu_k)|| \leq \tau_k$. *(At each step k we have to solve an unconstrained opt. problem: we use an iterative method so we need a starting point $\underline{x}_k^s$ and a stopping criterium)*

2.a If we satisfy the termination condition $|f(\underline{x}_k) - f(\underline{x}_{k-1})| < \epsilon$ then we return the solution $\underline{x}_k$.

2.b Otherwise we choose $\mu_{k+1} \in (0, \mu_k)$, the next starting solution $\underline{x}_{k+1}^{start}$ and we repeat from **1.**

- **Convergence.** If we guarantee that at every iteration k $\underline{x}_k$ is the global minimum of $Q(\underline{x}, \mu_k)$ and $\mu_k \to 0$ then every limit point $\underline{x}^*$ of $\{\underline{x}_k\}_k$ is a global minimum of the problem (P^1).
Anyway, the unconstrained problem is solved approximately. If $\tau_k \to 0$ and $\mu_k \to 0$ then every limit point $\underline{x}^*$ of $\{\underline{x}_k\}_k$ at which all $\nabla c_i(\underline{x}^*)$ are linearly independent is a KKT point of problem (P^1). So as limit point we get a candidate local optimal point. Moreover, for such points we have that $-\frac{c_i(\underline{x}_k)}{\mu_k} \to u_i^*$, $\forall i \in E$, where $\underline{u}^*$ satisfies with $\underline{x}^*$ the KKT conditions of (P^1). This result implies that the minimizer $\underline{x}_k$ of $Q(\underline{x}, \mu_k)$ does not satisfy $c_i(\underline{x}) = 0$, namely: $c_i(\underline{x}_k) = -\mu_k u_i^*$. Once again we see that μ_k must be driven to 0. The problem is that when $\mu_k \to 0$ the quadratic penalty problem becomes ill conditioned.
- **Equalities and inequalities.** The generic quaratic penalty problem for both eqality and inequality constraints is: $\min Q(\underline{x}, \mu) = f(\underline{x}) + \frac{1}{2\mu} \sum_{i \in E} c_i^2(\underline{x}) + \frac{1}{2\mu} \sum_{i \in I} ([c_i(\underline{x})]^-)^2$, where $[y]^- = \max\{-y, 0\}$.
- **Augmented Lagrangian method.** The augmented Lagrangian method reduces the ill-conditioning issue by introducing explicit estimates of the Lagrangian multipliers. For (P^1) we define the augmented Lagrange function $L_A(\underline{x}, \underline{u}, \mu) = f(\underline{x}) - \sum_{i=1}^m u_i c_i(\underline{x}) + \frac{1}{2\mu} \sum_{i=1}^m c_i^2(\underline{x})$, where $\underline{u}$ is the multiplier vector and μ is the penalty parameter. The general scheme is similar to the quadratic penalty method.

0. The method starts with a choice of an accuracy parameter ϵ, a starting penalty parameter μ_0 and a sequence of tolerances $\{\tau_k\}_k$. Moreover we choose a $\underline{x}_0^{start}$ and an initial multiplier vector $\underline{u}^0$

1. At the k-th iteration we determine an approximate minimizer $\underline{x}_k$ of $L_A(\underline{x}, \underline{u}^k, \mu_k)$ via an unconstrained optimization method. We stop when $||\nabla L_A(\underline{x}, \underline{u}^k, \mu_k)|| \leq \tau_k$.

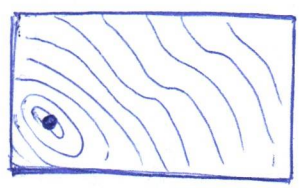
2.a If we satisfy $|f(\underline{x}_k) - f(\underline{x}_{k-1})| < \epsilon$ then we return the solution $\underline{x}_k$.

2.b Otherwise we set $u_i^{k+1} = u_i^k - \frac{c_i(\underline{x}_k)}{\mu_k}$, we choose $\mu_{k+1} \in (0, \mu_k)$, the next starting solution $\underline{x}_{k+1}^{start}$ and we repeat the procedure from **1.**

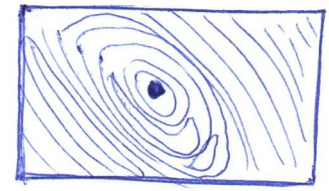
This method leads us to $c_i(\underline{x}_k) \approx \mu_k(u_i^k - u_i^*)$, which implies that we have two choices to obtain $c_i(\underline{x}_k) \to 0$ (i.e. equality constraints satisfied): either $\mu_k \to 0$, but we want to avoid it, or $u_i^k \to u_i^*$.

- **Example.** $\min \{x_1 + x_2 : x_1^2 + x_2^2 + 2 = 0\}$, with optimal solution $[-1, -1]^T$.

$$Q(\underline{x}, \mu) = \left[x_1 + x_2\right] + \left[\frac{1}{2\mu}\left(x_1^2 + x_2^2 - 2\right)^2\right]$$



$\mu = 1$



$\mu = 0.1$

The optimum is much closer here ($\mu = 0.1$) but the curves are becoming weirdly elongated (as $\mu \to 0$ the problem becomes ill conditionated)

Barrier method

Constrained Nonlinear Optimization

- We consider the problem (P): $\min \{f(\underline{x}) : c_i(\underline{x}) \geq 0 \;\; i \in I = \{1,..,m\}, \;\; \underline{x} \in \mathbb{R}^n\}$. We introduce the barrier function, a function defined on $\mathbb{R}^n$ and continuous over $X^o = int\{\underline{x} \in \mathbb{R}^n : c_i(\underline{x}) \geq \underline{0} \;\; i \in I\}$. The barrier function tends to ∞ when approaching the boundary of X and has value ∞ on $\mathbb{R}^n \setminus X^o$. The idea of the barrier method is to add to the objective function the barrier terms associated to the constraints and solve a sequence of resulting unconstrained optimization problems.
- For the problem (P) we define the logarithmic barrier problem: $\min P(\underline{x}, u) = f(\underline{x}) - \mu \sum_{i \in I} \ln c_i(\underline{x})$ with barrier parameter $\mu > 0$. If μ is a large value we're penalizing a lot the approach to the boundary, if $\mu \to 0$ we're decreasing the penalty of approaching and the barrier term becomes negligible.

0. We select an accuracy parameter $\epsilon > 0$, a starting penalty parameter $\mu_0 > 0$ and a sequence of tolerances $\{\tau_k\}_{k \geq 0}$ with $\tau_k \geq 0$ and $\tau_k \to 0$. We choose an initial point $\underline{x}_0^{start}$ and we set k=0.

1. Starting from $\underline{x}_k^{start}$ we determine an approximate minimizer $\underline{x}_k$ of $P(\underline{x}, \mu_k)$ with the stopping criterium: $||\nabla P(\underline{x}, \mu_k)|| \leq \tau_k$. *(At each step k we have to solve an unconstrained opt. problem: we use an iterative method so we need a starting point $\underline{x}_k^s$ and a stopping criterium)*

2.a If we satisfy the termination condition $|f(\underline{x}_k) - f(\underline{x}_{k-1})| < \epsilon$ then we return the solution $\underline{x}_k$.

2.b Otherwise we choose $\mu_{k+1} \in (0, \mu_k)$, the next starting solution $\underline{x}_{k+1}^{start}$ and we repeat from **1.**

Since $\underline{x}_0 \in X^o$ the sequence $\{\underline{x}_k\}_k$ remains in X^o, so the algorithm is an interior point method.

- Let $(\underline{x}^*, \underline{u}^*)$ satisfy the KKT conditions of (P), namely:

$$\nabla_{\underline{x}} L(\underline{x}, \underline{u}) = \nabla f(\underline{x}) - \sum_{i=1}^m u_i \nabla c_i(\underline{x}) = \underline{0} \tag{1}$$

$$-c_i(\underline{x}) \leq 0 \qquad \forall i \in I \tag{2}$$

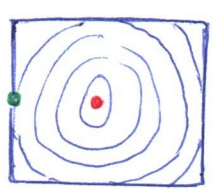
$$u_i c_i(\underline{x}) = 0 \qquad \forall i \in I \tag{3}$$

$$u_i \geq 0 \qquad \forall i \in I \tag{4}$$

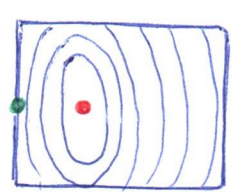
The minimizer $\underline{x}(\mu)$ of $P(\underline{x}, \mu)$ satisfies: $\nabla_{\underline{x}} P(\underline{x}, \mu) = \nabla f(\underline{x}) - \sum_{i=1}^m \frac{\mu}{c_i(\underline{x})} \nabla c_i(\underline{x}) = \underline{0}$. Combining the equations we obtain $u_i(\mu)\, c_i(\underline{x}(\mu)) = \mu$, which violates (3). When $\mu \to 0$ the minimum $\underline{x}(\mu)$ of $P(\underline{x}, \mu)$ and the corresponding estimate $u_i(\mu) = \frac{\mu}{c_i(\underline{x}(\mu))}$ tend to progressively satisfy the KKT conditions of (P).

- **Convergence.** If (1) $X^o \neq \emptyset$, $\underline{x}^*$ is a local minimum of (P) at which the KKT conditions are satisfied for some $\underline{u}^*$, (2) the gradients of the active constraints at $\underline{x}^*$ are linearly independent, (3) the strict complementary conditions are satisfied at $\underline{x}^*$ and (4) the 2nd sufficient conditions are satisfied at $(\underline{x}^*, \underline{u}^*)$ then $\exists!$ $\underline{x}(\mu)$ continuously differentiable vector function such that $\underline{x}(\mu) \to \underline{x}^*$ as $\mu \to 0^+$. For this $\underline{x}(\mu)$ the Lagrange multipliers estimates $\underline{u}(\mu)$ converge to $\underline{u}^*$ when $\mu \to 0^+$.
- If the problem has also equality constraints, we can include quadratic penalty terms, obtaining a combined log-barrier/quadratic penalty function problem. That's why the barrier method is seen as a "complementary" method to the quadratic penalty method.
- **Example.** $\min \{(x_1 - 0.5)^2 + (x_2 - 0.5)^2 : x_1 \in [0,1]^*, x_2 \in [0,1]\}$, $^* = \{x_1 \geq 0,\, 1 - x_1 \geq 0\}$.

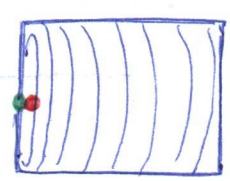
$$P(\underline{x}, \mu) = \left[(x_1 - 0.5)^2 + (x_2 - 0.5)^2\right] - \mu \left[\ln(x_1) + \ln(1 - x_1) + \ln(x_2) + \ln(1 - x_2)\right]$$



$\mu = 1$



$\mu = 0.1$



$\mu = 0.01$

- what we want
- what we get

Here the solution we get is good but the shape of the curves causes numerical problems